



## The finite - difference neutron diffusion programme TWODIM

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### The problem

The reactor model considered is a (not necessarily simply) connected bounded subset of  $R^2$  divided into a finite number of regions. Interfaces between regions, and the reactor boundary itself, consist of pieces of coordinate-surfaces in one of three geometries (xy, rz, or rθ). In each region the real functions  $D_g, \Sigma_{gg}, \Sigma_{p,g}, \chi_g, (\nu \Sigma_f)_g, S_g$  ( $1 \leq g, g' \leq ng$ ) are assumed constant and non-negative (the diffusion-coefficients  $D_g$  are assumed positive). In the reactor the neutron fluxes  $\phi_g$  ( $1 \leq g \leq ng$ ) satisfy the following system of partial differential equations

$$\begin{aligned}
 (1) \quad & -\nabla \cdot (D_g \nabla \phi_g) + \Sigma_{gg} \phi_g + \alpha \Sigma_{p,g} \phi_g = \\
 & = \sum_{g' \neq g} \Sigma_{gg'} \phi_{g'} + \lambda \chi_g \sum_{g'} (\nu \Sigma_f)_{g'} \phi_{g'} + S_g \\
 & \quad (1 \leq g \leq ng)
 \end{aligned}$$

$\alpha$  and  $\lambda$  are eigenvalues (see later).

Along the reactor boundary the so-called boundary regions must be specified. To each boundary-region corresponds a  $\gamma$ -matrix of order  $ng$ . At the interface between an ordinary region and the boundary-region the condition

$$(2) \quad -D_g \frac{\partial \phi_g}{\partial u} = \sum_{g'} \gamma_{gg'} \phi_{g'} \quad (1 \leq g \leq ng)$$

is applied;  $u$  is a coordinate with axis perpendicular to and out through the boundary. The  $\gamma$ -matrix must have non-negative diagonal elements and non-positive offdiagonal elements. Further  $\sum_{g'} \gamma_{gg'} \geq 0$  for all  $g$ . The latter condition, as well as the corresponding condition  $\sum_{g' \neq g} \Sigma_{g'g} \leq \Sigma_{gg}$ , combined with certain (usually trivially satisfied) connectedness-conditions on the set of supports for the coefficient-functions (see ref. 2) ensure existence and uniqueness of solution of the  $\lambda$ -eigenvalue problem.

There are 3 types of problems,

- 1)  $\lambda = 1/k_{\text{eff}}$  is a criticality-parameter ( $S_g = \Sigma_{p,g} = 0$ )
- 2)  $\alpha$  is a criticality-parameter ( $\lambda$  fixed,  $S_g = 0$ )
- 3) Sourceproblem ( $S_g \neq 0$ ,  $\lambda$  fixed,  $\Sigma_{p,g} = 0$ )

Similar techniques can be used for solving these problems.

#### Method of solution

Corresponding to the differential equations (1)+(2) we form in the usual way 5-point difference-equations in such a way that the Froehlich-conditions (ref. 2) are satisfied. The mesh-center discretization is used.

An "experimental" investigation of the convergence of the discrete solution towards the solution of (1)+(2) was reported in ref. 3, and one way of approaching the problem theoretically was indicated.

A special difficulty is connected with the correct representation of the boundary-conditions (2). They should be applied at the reactorboundary, but the difference-equations connect only fluxvalues at meshcenters. To avoid the necessity of superfine mesh in the vicinity of the boundary to keep discretization errors small the programme calculates a meshdependent  $\gamma$ -matrix (ref. 3), namely

$$(3) \quad \gamma_1 = \gamma \left( \frac{h}{2} D^{-1} \gamma + I \right)^{-1} = \left( I + \frac{h}{2} D^{-1} \right)^{-1} \gamma,$$

where D is the diagonal matrix (order ng) of diffusion-coefficients, while h is the meshwidth in the direction u.

We shall show that  $\gamma_1$  has the same properties as  $\gamma$ , namely

- a) it exists
- b) it has non-positive off-diagonal elements,
- c) its column-sums are non-negative (so that its diagonal elements must be non-negative too).

Introducing the following abbreviations,

$\underline{e}$  is a columnvector with all coordinates equal to one,

$$D_1 = \frac{h}{2} \bar{D}^{-1},$$

we see that the matrix  $I + \gamma D_1$  is strictly column diagonally dominant (for definitions and elementary theorems see ref. 4); in fact  $\underline{e}^T (I + \gamma D_1) \geq \underline{e}^T$ . Since its offdiagonal elements are nonpositive, its inverse exists and is nonnegative. This proves part a).

Part b) follows from the equation

$$\gamma_1 = (I + \gamma D_1)^{-1} \gamma = (I - (I + \gamma D_1)^{-1}) D_1^{-1}$$

and the remarks above.

To prove part c) we multiply the inequality  $\underline{e}^T (I + \gamma D_1) \geq \underline{e}^T$  from the right by the nonnegative matrix  $(I + \gamma D_1)^{-1}$ .

This gives  $\underline{e}^T (I - (I + \gamma D_1)^{-1}) \geq \underline{0}^T$ ,

$$\text{i.e. } \underline{e}^T \gamma_1 \geq \underline{0}^T \quad \text{and} \quad \underline{e}^T \gamma_1 \geq \underline{0}^T$$

The iterative scheme used in TWODIM for solution of the eigenvalueproblems is the so-called Equipoise - or neutron-balance-method (ref. 5), based on the SLOR-splitting. In ref. 6 examples were given of cyclic divergence with this scheme for regular splittings and for some matrices satisfying the Froehlich-conditions. These examples did not even show local convergence (i.e. convergence with a start-vector arbitrarily situated within a sufficiently small distance from the solution). Some work has been done to further investigate conditions for local convergence, but nothing of practical value has come out of this. It seems that the method converges for all cases which are not specifically contrived to demonstrate divergence. Some instances of very slow convergence have been found, however, and in such cases the TWODIM-programme automatically switches to more than 1 inner iteration per outer.

To accelerate convergence the programme uses extrapolation as soon as the estimated convergence-rate for the SLOR-iterations meets a user-specified criterion for convergence.

The Equipoise-scheme has been compared to another one (in the following denoted the DC3-scheme after the programme (ref. 7), where it was first used). Here the eigenvalue is calculated as the Rayleigh-quotient corresponding to the current flux-iterate. The DC3-method is really a rather general method, which can be applied to self-adjoint eigenvalue-problems

$$(4) \quad \langle \phi | = \lambda M \phi,$$

where the operator  $M$  is positive semi-definite (see ref. 8). A sequence of vectors  $\phi_n$  ( $n \in \mathbb{N}$ ) is generated, for which the corresponding eigenvalue-estimates form a decreasing sequence. With certain precautions one can demonstrate convergence towards the smallest eigenvalue. Specific applications and/or comparisons with other methods have been described in refs. 9-14. The DC3-programme was sent to the Ispra-library in 1964 but has, apparently, not been used. We did not use it at Risø after 1964, since the Equipoise-scheme is simpler. And for problems with more than one energy-group there is no reason to prefer the DC3-scheme, since the flux is usually not a better approximation to the adjoint flux than the constant distribution  $e$  is. One of the options in the DC4-programme (ref. 15) consists in using the generalized Rayleigh-quotient with a periodically updated adjoint-fluxestimate. However, also this scheme was found to be too complicated compared to the Equipoise-method.

#### Input

The following description is partly taken from ref. 16.

In the input-list below two consecutive logical records are separated by a horizontal line. A logical record may consist of several physical records (cards), but a shift of logical record implies shift of card.

All items of the input occur in the output too (see the sample problem).

Name of inputfile: d2di

Name of restart-(disk-)file: tworest

Input-list

Name	type	meaning
problem	integer	problem-number
geom	integer	geometry, 1=xy, 2=rz, 3=r $\theta$
cmx	-	number of material mesh regions in x-direction
cmx	-	- - - - - y -
ncp	-	number of materials ("boundary materials" inclusive)
nb	-	number of boundary materials
ndb	-	- - - - - with $\gamma$ diagonal
ng	-	number of energy groups
nthg	-	- - thermal groups (possibly with upscattering)
type	-	calculation-type, 1= $\lambda$ , 2= $\alpha$ , 3=source
nrec	-	number of recalculations (with mesh refinement)
prev	-	if prev>0 initial flux and eigenvalues are read from the disk-file tworest (coarse mesh only). For every abs (prev) iterations eigenvalues and fluxiterate are written on tworest (finest mesh only)
rela	-	direction of lines in SLOR, 2=x, 3=y
mx	integer	number of regions (finest mesh) for x-direction
my	integer	- - - - - y -
xc	array	material mesh x line coordinates
		[0:cmx]



Name	type	meaning
fmx	integer array [1:cmx]	for each material mesh in x-direction number of coarse mesh regions
facx	integer array [1:cmx]	(only for nrec>0) mesh refinement factor for each material mesh in x-direction (applied for each recalculation)
yc	array [0:cmx]	as xc, but for y-direction; for r0 - geometry 0 must be in radians
fmy	integer array [1:cmx]	as fmx, but for y-direction
facy	integer array [1:cmx]	(only for nrec>0); as facx, but for y-direction
cpnc	integer array [0:cmx+1, 0:cmx+1]	map of material numbers (including interior and exterior boundary materials), each logi- cal record consisting of a row (cmx+2 numbers), starting with the row corresponding to the last read y-values. Note that a complete rectangular set of numbers must be specified. Those numbers which are meaningless (for instance in case of large internal control areas or corner-regions) should be boundary material numbers
f	integer	format-indicator for the following multi- group-coefficients: 1=6el2,5, otherwise free format

The following set of records specifies data for each material. As regards notation see eq. (1).

name	type	meaning
k	integer	material number or 0; what data are expected after this, depends on k
gad	array [1:ng]	diagonal $\gamma$ -matrix (for $0 < k \leq \text{ndb}$ )
gam	array [1:ng, 1:ng]	$\gamma$ -matrix (for $\text{ndb} < k \leq \text{nb}$ )
dd	array [1:ng]	$D_g$
ss	array [1:ng, 1:ng]	$\Sigma_{g,g'}$
fs	array [1:ng]	$\chi_g$
nsf	-	$(v\Sigma_f)_g$
rr	-	reactionrate-(usually fission-) cross sections (see sample output)
pp	-	(only for type $\neq 1$ ) for type = 2: $\Sigma_{p,g}$ for type = 3: $S_g$
kb	integer	For material numbers $m \in [kb, ke]$
ke	-	(k=0 only) the data are set equal to those just read

(for  $\text{nb} < k \leq \text{ncp}$ )

The number of non-zero k-values plus the sum of the numbers  $(ke - kb + 1)$  must equal  $\text{ncp}$ .

The following control-variables (rm to kappa incl.) have default-values, obtained, if the input-value is negative. They are given in parentheses in the following list.

If the recommended value differs from the default-value, it is given in a second parenthesis.

name	type	meaning
rm	integer	maximum iteration number (50)
rb	-	number of initial iterations before calculation of extrapolation parameter begins (3)
re	-	number of consecutive iterations in which the estimated convergence-rate must have a relative deviation less than epse before extrapolation (3)
rd	-	number of iterations after extrapolation before calculation of new extrapolation parameter starts (3)
eps	real	the iterations stop when the estimated rms-error in the flux-distribution is less than eps times maximal flux (0.0001)
epsm	-	the overrelaxation-factor omega is altered when the estimated convergence-rate has converged within epsm (see above under re) (0)
epse	-	see under re above (0.5)(0.1)
omega	-	overrelaxation-factor (1.2) (1.5)
lamb	-	$\lambda = 1/k_{eff}$ (1)
alfa	-	$\alpha$ (1)
kappa	-	$\kappa$ = upper bound for $\alpha$ . The internal eigenvalue-parameter for type 2-calculations is $\kappa - \alpha > 0$ (1)
printer	integer	For printer < 2 only the eigenvalues are printed; for $2 \leq \text{printer} < 9$ flux- and reaction-rate-distributions are printed, too; for printer $\geq 9$ the print-out contains also progress-report for the iterations

For each calculation (nrec + 1 times in all) the following set of input parameters must be specified:

name	type	meaning
powerout	integer	powerout < - 2 gives no reaction-rate-printout (if all reaction-rate-crosssections are zero there is no reaction-rate-printout either); if power=-1 the reaction-rate-distribution is calculated and printed for the earlier specified grid (initially the coarse grid); if powerout=-2 a new grid must be specified (see below)
facxp	integer array [0:mx]	(for powerout=-2) mx is the number of regions in the current mesh; facxp[n]=1 means that x-interface-line number n+1 in the current mesh shall also be an interface-line in the reaction-rate-grid
facyp	integer array [0:my]	(for powerout = -2) as facxp (mutatis mutandis)

### Output

As seen in the samp'e-output the input is printed immediately after it has been read.

The amount of output is governed by the input-parameter printer, as described above, and may contain progress-report for the iterations, flux- and reaction-rate-(usually power-density-) tables.

References

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16. C.F. Højerup, Risø, Denmark, unpublished work (1971).

PROBLEM

GEOM 1. CMX 3. CMY 3. VCP 6. NB 2. NDB 1. NG NTFG TYPE NREC PREV RELA  
 MX 16. MY 16.

XC 0. 6.000E+00 7.000E+00 8.000E+00

FMX 6. 1. 1.

FACX 2. 2. 2.

YC 0. 6.000E+00 7.000E+00 8.000E+00

FMY 6. 1. 1.

FACY 2. 2. 2.

COMPOSITION NUMBERS

1. 2. 2. 2. 2.

1. 3. 3. 3. 3.

1. 5. 5. 5. 5.

1. 4. 4. 4. 4.

1. 1. 1. 1. 1.

COMPOSITIONS

EFORMAT= 0

1 EXTPL: 0. 0.

2 GAM: 2.000E-01 0. -1.000E-01 5.000E-02

3 D: 2.000E+00 3.000E-01

SS: 3.000E-02 0. 3.000E-02 1.000E-02

FS: 1.000E+00 0.

NSF: 0. 0.

RR/SF: 0. 0.

4 D: 1.000E+00 4.000E-01

SS: 2.000E-02 0. 1.000E-02 1.000E-02

FS: 1.000E+00 0.

NSF: 0. 5.000E-02

RR/SF: 0. 2.000E-02

0

5 6 RP RB RE RD EPS EPSM EPSE OMEGA

-1.0000E+00 -1.0000E+00 -1.0000E+00 -1.0000E+00 -1.0000E+00 -1.0000E+00 -1.0000E+00 -1.0000E+00

-1.0000E+00 -1.0000E+00 -1.0000E+00

PRINTER= 16.  
 KEFF CALCULATION

TWODIM sample output.





```
FLUX
Y I I
GROUP 1.
7500. 5412. 3256. 5323. 4716. 4344. 1036. 3569.
6500. 6423. 5241. 5965. 5593. 5118. 4224. 3936.
5500. 7592. 7077. 6747. 6403. 5996. 5118. 4344.
4500. 8326. 8032. 7766. 7135. 6493. 5193. 4716.
3500. 8757. 8691. 8279. 7706. 6247. 5065. 5023.
2500. 5412. 5129. 4691. 3092. 7377. 5241. 5258.
1500. 9707. 8412. 8357. 8325. 7492. 5423. 5412.
9999. 9851. 9551. 9384. 8445. 7598. 5914. 5489.

--- X 500.1500.2500.3500.4500.5500.6500.7500.
Y I I
GROUP 2.
7500. 9517. 9408. 9253. 9054. 8850. 8645. 8431.
6500. 9302. 9260. 9191. 9071. 8944. 8812. 8645.
5500. 9131. 9149. 9090. 9011. 8925. 8852. 8645.
4500. 9112. 9108. 9064. 9004. 8956. 8925. 8645.
3500. 9124. 9106. 9073. 9076. 9008. 9011. 9071. 9253.
2500. 9136. 9122. 9098. 9073. 9064. 9090. 9181. 9403.
1500. 9152. 9140. 9122. 9106. 9108. 9149. 9260. 9516.
9162. 9152. 9136. 9124. 9132. 9181. 9202. 9573.

--- A 500.1500.2500.3500.4500.5500.6500.7500.
REACTION RATE DENSITY
CALCULATION NUMBER 1
POWEROUT
-2
FACXP 1 0 1 0 1 0 1 0 1
FACYP 1 0 1 0 1 0 1 0 1
Y I I
AVERAGE 10000
7000. 5111 5026 4890 2398
5000. 10070 9961 9819 4890
3000. 10047 9930 9951 5026
1000. 10030 10048 10070 5111

--- X 1000. 3000. 5000. 7000. 5.1 I/O.TIME= 0.7
EL.TIME= 8.4 PROC.TIME=
```

[illegible]

FLY I

[illegible]

Y I I	GROUP 2.
7750.	9595.9580.9550.9506.9449.9378.9296.9203.9102.8995.8882.8768.8652.8537.8418.8293.
7250.	9486.9473.9447.9409.9359.9298.9228.9150.9065.8976.8884.8791.8703.8614.8522.8418.
6750.	9347.9136.9314.9281.9239.9187.9128.9063.8994.8922.8851.8782.8718.8663.8614.8537.
6250.	9260.9250.9230.9202.9165.9121.9070.9016.8958.8900.8844.8792.8749.8718.8703.8653.
5750.	9177.9189.9172.9147.9115.9077.9034.8989.8942.8896.8853.8818.8793.8782.8793.8768.
5250.	9155.9148.9133.9111.9084.9052.9016.8978.8940.8905.8875.8854.8844.8851.8885.8881.
4750.	9129.9122.9110.9091.9067.9040.9010.8979.8950.8924.8905.8896.8900.8921.8976.8995.
4250.	9115.9109.9098.9082.9062.9039.9014.8990.8968.8950.8940.8942.8958.8994.9065.9103.
3750.	9110.9105.9095.9081.9064.9045.9025.9006.8990.8980.8978.8989.9016.9064.9150.9204.
3250.	9111.9107.9098.9086.9072.9055.9039.9025.9014.9010.9016.9035.9071.9129.9228.9296.
2750.	9116.9113.9105.9095.9082.9068.9055.9045.9039.9040.9052.9077.9121.9188.9299.9378.
2250.	9121.9120.9113.9104.9093.9082.9072.9064.9062.9068.9084.9115.9163.9239.9359.9449.
1750.	9131.9128.9122.9114.9104.9095.9086.9081.9082.9091.9111.9147.9202.9282.9409.9507.
1250.	9132.9135.9129.9122.9113.9105.9098.9095.9098.9110.9133.9172.9231.9314.9448.9551.
750.	9143.9140.9135.9128.9120.9113.9107.9105.9109.9122.9148.9189.9250.9336.9473.9580.
250.	9145.9143.9138.9131.9123.9116.9111.9110.9115.9129.9155.9197.9260.9348.9486.9595.

---- X 250. 750. 1250. 1750. 2250. 2750. 3250. 3750. 4250. 4750. 5250. 5750. 6250. 6750. 7250. 7750.  
REACTION RATE DENSITY

# CALCULATION NUMBER 2

POWEROUT

Y I I	AVERAGE 10000
7000.	5115 5030 4896 2401
5000.	10069 9971 9824 4896
3000.	10040 9945 9951 5030
1000.	10069 10040 10069 5115

---- X 1000. 3000. 5000. 7000.  
EL.TIME= 29.1 PRIC.TIME= 19.6 I/O.TIME= 1.0